

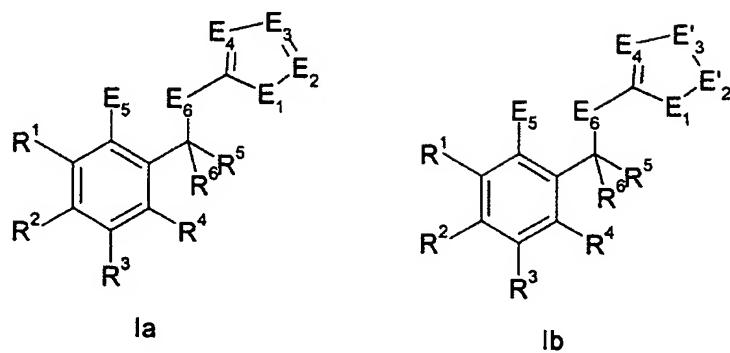
BASF Aktiengesellschaft

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We claim:

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1. A compound of the formula Ia or Ib



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where,

in the formula Ia,

E1 is O, S, Se, Te, NR, CR₂, PR,

E2, E3 are each CR, N, P,

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E4 is N, P,

E5 is OH, SH, NHR, or OR', SR', NRR',

E6 is NH, PH, or NR', PR',

R^5, R^6 are each hydrogen or a linear, branched or cyclic alkyl radical or an aryl radical,

20 R^1, R^2, R^3, R^4 are each hydrogen, a linear, branched or cyclic alkyl radical, an aryl radical, a halogen or a nitro group,

R is hydrogen, a linear, branched or cyclic alkyl radical,

R' is a linear, branched or cyclic alkyl radical,

where at least one of the groups E5 and E6 contains a hydrogen atom;

25

in the formula Ib.

the symbols E_1 , E_4 , E_5 , E_6 , R^5 , R^6 , R^1 , R^2 , R^3 , R^4 , R and R' are as defined in formula 1a

and

E2' and E3' are each O, S, Se, Te, NR, CR₂, PR.

2. A compound as claimed in claim 1, wherein E1 is S.

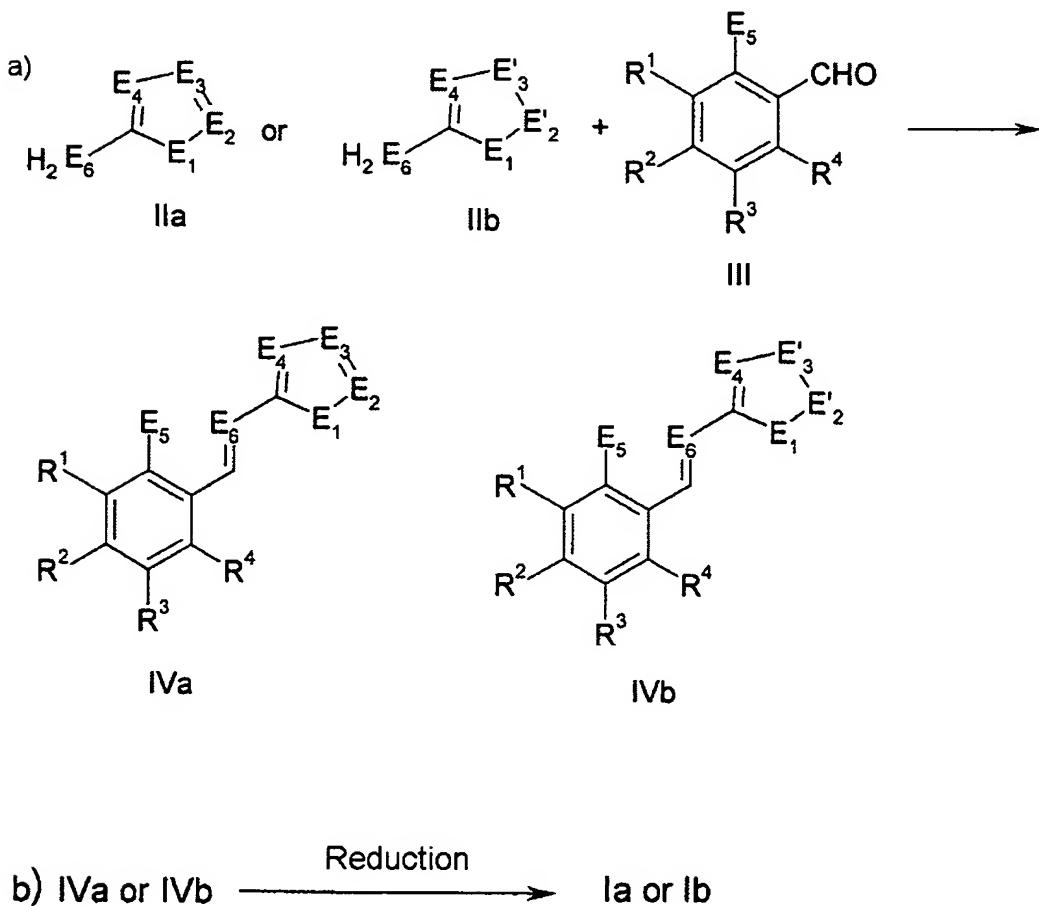
3. A compound as claimed in claim 1 or 2, wherein E4 is N.

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4. A compound as claimed in any of claims 1 to 3, wherein E6 is NH.

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5. A process for preparing a compound as claimed in any of claims 1 to 4, which comprises reacting a compound of the formula IIa or IIb with a compound of the formula III to form a compound of the formula IVa or IVb (step a)) and subsequently reducing the compound of the formula IVa or IVb to give a compound of the formula Ia or Ib (step b)):



where

E1 is O, S, Se, Te, NR, CR₂, PR, preferably S,
 E2, E3 are each CR, N, P,
 5 E2', E3' are each O, S, Se, Te, NR, CR₂, PR,
 E4 is N, P, preferably N,
 E5 is OH, SH, NHR, or OR', SR', NRR',
 E6 is NH, PH, preferably NH, or NR', PR',
 R⁵, R⁶ are each hydrogen or a linear, branched or cyclic alkyl radical or an
 10 aryl radical,
 R¹, R², R³, R⁴ are each hydrogen, a linear, branched or cyclic alkyl radical, an aryl
 radical, a halogen or a nitro group,
 R is hydrogen, a linear, branched or cyclic alkyl radical,
 R' is a linear, branched or cyclic alkyl radical,
 15 where at least one of the groups E5 and E6 contains a hydrogen atom.

6. The use of a compound as claimed in any of claims 1 to 4 for preparing metal complexes.

20 7. A metal complex of the formula V



where

L is a monoanionic or dianionic ligand derived from a compound of the
 25 formula Ia or Ib as claimed in any of claims 1 to 4

where,

- in the case of a dianionic ligand,

E5 is O⁻, S⁻, RN⁻, preferably O⁻, and

E6 is N⁻, P⁻, preferably N⁻,

30 and, in the case of a monoanionic ligand,

either

E5 is O⁻, S⁻, RN⁻, preferably O⁻, and

E6 is NR, PR

or

35 E5 is OR, SR, NRR', and

E6 is N, P, preferably N,

and the further symbols E1, E2, E2', E3, E3', E4, R⁵, R⁶, R¹, R², R³, R⁴, R and R' in the formulae I and II have the same meanings as forth for the corresponding symbols in any of claims 1 to 4;

5 and, when L is a dianionic ligand,

M is Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, preferably Ti, Zr, Hf,

R" is hydrogen, a hydrocarbon radical, preferably a linear, branched or cyclic alkyl radical, NR"₂, OR", halogen, acetylacetone, preferably halogen, OR", where R" is hydrogen or a linear, branched or cyclic alkyl radical,

10 Y is a Lewis base,

x is 1 or 2, preferably 1,

y is from 1 to 4, preferably 2,

z is from 0 to 2, preferably 0

where R" and Y may be joined to form a joint radical and 2x + y corresponds to the 15 valence of M;

or, when L is a monoanionic ligand,

M is Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Ni, Pd, Co, Fe, Cu, Ru, Rh, preferably Ti, Zr, Hf, Ni, Pd,

R" is hydrogen, a hydrocarbon radical, preferably a linear, branched or cyclic alkyl radical, NR"₂, OR", halogen, acetylacetone, preferably halogen, OR", where R" is hydrogen or a linear, branched or cyclic alkyl radical,

20 Y is a Lewis base,

x is 1, 2 or 3,

y is from 1 to 4,

25 z is from 0 to 2, preferably 0,

where R" and Y may be joined to form a joint radical and x + y corresponds to the valence of M.

8. A metal complex as claimed in claim 7, wherein the ligand L is a dianionic ligand 30 and M is Ti, Zr or Hf.

9. A metal complex as claimed in claim 8, wherein x is 1, y is 2 and z is 0.

10. A metal complex as claimed in claim 7, wherein the ligand L is a monoanionic 35 ligand and M is Ti, Zr, Hf, Ni or Pd.

11. A metal complex as claimed in claim 10, wherein when M is Ti, Zr, Hf, x is 2, y is 2 and z is 0 or x is 1, y is 3 and z is 0 and when M is Ni or Pd, x is 1, y is 1 and z is 0.

5 12. A process for preparing a metal complex as claimed in any of claims 7 to 11 by deprotonation of a compound as claimed in any of claims 1 to 4 by means of a base and subsequent reaction with a metal compound, or by direct reaction of a compound as claimed in any of claims 1 to 4 with a metal compound,

10 where the metal compound comprises a metal M selected from the group consisting of Ti, Zr, Hf, V, Nb, Ta, Cr, Mo and W, preferably Ti, Zr, Hf, when L is a dianionic ligand, or a metal M selected from the group consisting of Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Ni, Pd, Co, Fe, Cu, Ru and Rh, preferably Ti, Zr, Hf, Ni, Pd, when L is a monoanionic ligand.

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13. A catalytically active composition comprising

- a) a metal complex of the formula V as claimed in any of claims 7 to 11 as component A,
- b) at least one compound, as component B, selected from the group consisting of
 - (b1) an organometallic compound, as component B1,
 - (b2) an organoaluminum oxy compound, as component B2, and
 - (b3) a compound which reacts with the metal complex to form an ion pair, as component B3.

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14. A catalytically active composition as claimed in claim 13 which further comprises a support material (component C) in addition to the components A and B.

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15. A process for preparing a catalytically active composition as claimed in claim 13 or 14, which comprises bringing a metal complex of the formula V as claimed in any of claims 7 to 11 (component A) into contact with a compound (component B) selected from the group consisting of

- (b1) an organometallic compound, as component B1,

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(b2) an organoaluminum oxy compound, as component B2, and
(b3) a compound which reacts with the metal complex to form an ion pair, as component B3,
and optionally a support material (component C).

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16. The use of a catalytically active composition as claimed in claim 13 or 14 for the polymerization or copolymerization of olefins.

10 17. A process for the polymerization or copolymerization of olefins, which comprises polymerizing an olefin in the presence of a catalytically active composition as claimed in claim 13 or 14 or copolymerizing at least two different olefins in the presence of a catalytically active composition as claimed in claim 13 or 14.

15 18. A polymer or copolymer which can be prepared by a process as claimed in claim 17.